Note Regarding MLE and Asymmetries

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Abstract

This document discusses in which case Maximum Likelihood Estimation (MLE) extracts azimuthal moments or azimuthal asymmetries. This document is an extension of an email by A. Miller [1] linked from the HERMES Wiki page on fitting [2]. This document also continues past Andy's email, to determine the effect of including acceptance corrections [3] and discusses the proper interpretation when using the Monte Carlo Normalization and Weighting methods. The Monte Carlo Normalization is found to have limited interpretability, while the Weighting method is broadly applicable and more easily interpreted.

1 MLE Azimuthal Moment Extaction

For example, consider fitting a transverse target data set. Without loss of generality, we can separate the $(D+2)$-dimensional differential cross section into the polarized and unpolarized sections,

$$\sigma_\pm = \sigma_{UU}(\boldsymbol{x},\phi) \pm \sigma_{UT}(\boldsymbol{x},\phi,\phi_s), \tag{1}$$

where $\boldsymbol{x}$ represents the D-tuple of kinematic variables. Also without loss of generality, one can expand the unpolarized term in Fourier moments,

$$\sigma_{UU}(x,\phi) = A^0_{UU}(\boldsymbol{x}) + \sum_{n=1}^{\infty} A^{\cos(n\phi)}_{UU}(\boldsymbol{x})\cos(n\phi), \tag{2}$$

and also factor the angular integrated portion, A^0_{UU}, from the other moments of the cross section

$$\sigma_\pm = A^0_{UU}(\boldsymbol{x})\left[W_{UU}(\boldsymbol{x},\phi) \pm W_{UT}(\boldsymbol{x},\phi,\phi_s)\right]. \tag{3}$$

1.1 Asymmetry Moments

Consider data distributed according to the above cross section, and fit using MLE and the function

$$p_\pm \propto 1 \pm p_{UT}(\phi,\phi_s) \tag{4}$$

with

$$p_{UT}(\phi,\phi_s) = a\sin(\phi_s) + \ldots. \tag{5}$$

Following A. Miller's email, we consider the limit of infinite statistics, where the sums in the MLE divided by the number of statistics converge to the integral

$$L = \int d^D\boldsymbol{x}d\phi d\phi_s\ \left[\sigma_+ \ln p_+ + \sigma_- \ln p_-\right]. \tag{6}$$

Taking the derivative with respect to the parameter a yields

$$\begin{aligned}
0 &= \frac{\partial L}{\partial a}, & (7)\\
&= \int d^D\boldsymbol{x}d\phi d\phi_s\ \left[\frac{\sigma_+}{p_+} - \frac{\sigma_-}{p_-}\right]\sin\phi_s, & (8)\\
&= \int d^D\boldsymbol{x}d\phi d\phi_s\ \left[\frac{W_{UU}(\boldsymbol{x},\phi)+W_{UT}(\boldsymbol{x},\phi,\phi_s)}{1+p_{UT}(\phi,\phi_s)} - \frac{W_{UU}(\boldsymbol{x},\phi)-W_{UT}(\boldsymbol{x},\phi,\phi_s)}{1-p_{UT}(\phi,\phi_s)}\right] A^0_{UU}(\boldsymbol{x})\sin\phi_s, & (9)\\
&= 2\int d^D\boldsymbol{x}d\phi d\phi_s\ \Big[W_{UT}(\boldsymbol{x},\phi,\phi_s) - W_{UU}(\boldsymbol{x},\phi)p_{UT}(\phi,\phi_s)\Big] A^0_{UU}(\boldsymbol{x})\frac{\sin\phi_s}{1-p^2_{UT}(\phi,\phi_s)}. & (10)
\end{aligned}$$

Integrating over $\boldsymbol{x}$ yields

$$0 \;=\; 2\int d\phi d\phi_s \, \left[\langle W_{UT}\rangle - \langle W_{UU}\rangle \, p_{UT}(\phi,\phi_s)\right] \frac{\sin\phi_s}{1-p_{UT}^2(\phi,\phi_s)}, \tag{11}$$

where, as usual, the average is with respect to the kinematic variables and the angular-integrated cross section,

$$\langle f(\boldsymbol{x})\rangle = \int d^D\boldsymbol{x} A^0_{UU}(\boldsymbol{x}) f(\boldsymbol{x}). \tag{12}$$

The maximum likelihood is then obtained when

$$p_{UT} = \frac{\langle W_{UT}\rangle}{\langle W_{UU}\rangle} = \frac{\sigma_+ - \sigma_-}{\sigma_+ + \sigma_-}. \tag{13}$$

1.2 Amplitudes

Going through the same exercise with

$$p_\pm \;\propto\; p_{UU}(\phi) \pm p_{UT}(\phi,\phi_s), \tag{14}$$

$$p_{UU}(\phi) \;=\; 1 + b\cos(\phi) + \ldots \tag{15}$$

yields the solution

$$p_{UU} \;=\; \langle W_{UU}\rangle = \int d\boldsymbol{x}\; A^0_{UU}(\boldsymbol{x}) W_{UU}(\boldsymbol{x},\phi,\phi_s), \tag{16}$$

$$p_{UT} \;=\; \frac{\langle W_{UT}\rangle}{\langle W_{UU}\rangle} p_{UU} = \langle W_{UT}\rangle = \int d\boldsymbol{x}\; A^0_{UU}(\boldsymbol{x}) W_{UT}(\boldsymbol{x},\phi,\phi_s). \tag{17}$$

Thus if one fits or correctly inputs the angular unpolarized cross section, then indeed the amplitudes are extracted. However, if one does not include the angular unpolarized moments in the fit function, then indeed the asymmetry is extracted.

2 Acceptance Corrections: Normalization Monte Carlo Method

The full differential yield has the form

$$\begin{aligned} dN_\pm(\boldsymbol{x},\phi,\phi_s) &= L_\pm\; \epsilon(\boldsymbol{x},\phi,\phi_s)\; \left(\sigma_{UU}(\boldsymbol{x},\phi) \pm \sigma_{UT}(\boldsymbol{x},\phi,\phi_s)\right) \\ &= L_\pm\; \epsilon(\boldsymbol{x},\phi,\phi_s)\; A^0_{UU}(\boldsymbol{x})\; \left[W_{UU}(x,\phi) \pm W_{UT}(\boldsymbol{x},\phi,\phi_s)\right], \end{aligned} \tag{18}$$

where the new quantities are the luminosity for each polarization state $L_\pm$, and the acceptacne function $\epsilon(\boldsymbol{x},\phi,\phi_s)$.

Consider using the fit function $f_\pm$ defined as

$$f_\pm(\phi,\phi_s) \;=\; L_\pm\; \langle \epsilon(\boldsymbol{x},\phi,\phi_s)\rangle \, p_\pm(\phi,\phi_s), \tag{19}$$

where $p_\pm$ is thus far unspecified. Note

$$\langle \epsilon(\boldsymbol{x},\phi,\phi_s)\rangle = \int d^D\boldsymbol{x} A^0_{UU}(\boldsymbol{x})\epsilon(\boldsymbol{x},\phi,\phi_s) \tag{20}$$

is a function of ϕ and ϕ_s. Let

$$F_\pm = \int d\phi d\phi_s\; f_\pm(\phi,\phi_s). \tag{21}$$

As described in Reference [3], the quantity $L_\pm\,\langle\epsilon\rangle$ constributes a constant to the log-likelihood (which does not affect the maximum), and also enters into the normalization integral of $f_\pm$. This normalization integral can be estimated (up to a constant) using Monte Carlo data, hence the common phrase of "using normalization Monte Carlo" meaning that one is correcting for the acceptance in this manner.

The log-likelihood can be written

$$L = \sum_{i=1}^{n_+} \ln \frac{p_+(\phi_+^{(i)}, \phi_{s+}^{(i)})}{F_+} + \sum_{j=1}^{n_-} \ln \frac{p_-(\phi_-^{(j)}, \phi_{s-}^{(j)})}{F_-} + \text{const.} \tag{22}$$

In the limit of infinite statistics ($n^+ = n^- = n \to \infty$), this becomes

$$\frac{L}{n} \propto \int d^D\boldsymbol{x} d\phi d\phi_s \ \left[\frac{dN_+}{\int dN_+} \ln \frac{p_+}{F_+} + \frac{dN_-}{\int dN_-} \ln \frac{p_-}{F_-} + \right]. \tag{23}$$

In contrast to the first section, where the asymmetry was considered before the amplitude (allowing the most directly comparison with the email of Andy Miller), this section begins with the amplitudes, as the presentation is cleaner.

2.1 Amplitudes

Let $p_\pm$ be defined according to Equations 14, 15. Taking the derivative with respect to the parameter b yields

$$\begin{aligned} 0 &= \frac{\partial L}{\partial b} && (24) \\ &\propto \int d^D\boldsymbol{x} d\phi d\phi_s \ \left\{\left(\frac{dN_+}{\int dN_+}\frac{1}{p_+} + \frac{dN_-}{\int dN_-}\frac{1}{p_-}\right)\cos\phi \right. \\ &\quad \left. - \left(\frac{dN_+}{\int dN_+}\frac{L_+}{F_+} + \frac{dN_-}{\int dN_-}\frac{L_-}{F_-}\right)\left[\int d\phi' d\phi_s' \ \langle \epsilon(\boldsymbol{x}, \phi', \phi_s')\rangle \cos\phi'\right]\right\} && (25) \\ &\propto \left\{\int d^D\boldsymbol{x} d\phi d\phi_s \ \left(\frac{dN_+}{\int dN_+}\frac{1}{p_+} + \frac{dN_-}{\int dN_-}\frac{1}{p_-}\right)\cos\phi\right\} \\ &\quad - \left(\frac{L_+}{F_+} + \frac{L_-}{F_-}\right)\int d\phi' d\phi_s' \ \langle \epsilon(\boldsymbol{x}, \phi', \phi_s')\rangle \cos\phi'. && (26) \end{aligned}$$

Since the second line in the above equation is non-zero in general, the solution requires

$$\begin{aligned} 0 &= \frac{1}{\int dN_\pm}\int d^D\boldsymbol{x} d\phi d\phi_s \ \cos(\phi)\ \frac{dN_\pm}{p_\pm} - \frac{L_\pm}{F_\pm}\int d\phi' d\phi_s' \ \langle \epsilon(\boldsymbol{x}, \phi', \phi_s')\rangle \cos\phi' && (27) \\ &\propto \frac{1}{\int dN_\pm}\int d\phi d\phi_s \ \cos(\phi) \ \int d^D\boldsymbol{x} \ \epsilon(\boldsymbol{x}, \phi, \phi_s) A_{UU}^0(\boldsymbol{x}) \frac{W_{UU}(\boldsymbol{x}, \phi) \pm W_{UT}(\boldsymbol{x}, \phi, \phi_s)}{p_{UU}(\phi) \pm p_{UT}(\phi, \phi_s)} \\ &\quad - \frac{1}{F_\pm}\int d\phi d\phi_s \ \cos(\phi) \ \int d^D\boldsymbol{x} \ \epsilon(\boldsymbol{x}, \phi, \phi_s) A_{UU}^0(\boldsymbol{x}). && (28) \end{aligned}$$

Equivalently, taking the derivative with respect to the parameter a yields

$$\begin{aligned} 0 &= \frac{\partial L}{\partial a} && (29) \\ &\propto \left\{\int d^D\boldsymbol{x} d\phi d\phi_s \ \left(\frac{dN_+}{\int dN_+}\frac{1}{p_+} - \frac{dN_-}{\int dN_-}\frac{1}{p_-}\right)\sin(\phi_s)\right\} \\ &\quad - \left(\frac{L_+}{F_+} - \frac{L_-}{F_-}\right)\int d\phi d\phi_s \ \langle \epsilon(\boldsymbol{x}, \phi, \phi_s)\rangle \sin(\phi' - \phi_s'). && (30) \end{aligned}$$

In general, it is not obvious whether each polarization state should cancel separately, as was the case for the derivative with respect to b, or whether the two states cancel against each other. If the detector is even with respect to ϕ_s (i.e. top-bottom symmetric), then $(L_+/F_+ - L_-/F_-) = 0$ and $\int dN_+ = \int dN_-$, since p_{UT} and W_{UT} are odd with respect to ϕ_s. Equation 29 reduces to

$$0 = \int d^D\boldsymbol{x} d\phi d\phi_s \left(\frac{dN_+}{p_+} - \frac{dN_-}{p_-}\right)\sin(\phi_s) \tag{31}$$

$$\propto \int d\phi d\phi_s \; \sin(\phi_s) \int d^D\boldsymbol{x}\; \epsilon(\boldsymbol{x},\phi,\phi_s) A^0_{UU}(\boldsymbol{x}) \frac{W_{UT}(\boldsymbol{x},\phi,\phi_s)p_{UU}(\phi) - W_{UU}(\boldsymbol{x},\phi,\phi_s)p_{UT}(\phi,\phi_s)}{p_{UU}(\phi)^2 - p^2_{UT}(\phi,\phi_s)}. \tag{32}$$

In both cases, the solution yet contains the acceptance in non-trivial ways, and thus this method has not corrected for acceptance, only changed somewhat how the acceptance enters. Note, if the data were binned sufficiently fine in $\boldsymbol{x}$, (i.e. is sufficiently fine in all relevant kinematic variables) then the solution does not depend on acceptance. However, and quite unfortunately, the interpretation of the results does depend on how fine the binning is. If the binning is such that the acceptance is approximately constant over the entire kinematic integration range, (with respect to all kinematic variables) and yet A^0_{UU}, W_{UU} and W_{UT} are not constant, then the acceptance can effectively be taken out of the integral and replaced by its average value. The other terms stay in the integral, and the solution is again that of Equations 16 and 17.

If instead the binning is such that W_{UU} and W_{UT} are approximately constant with respect to all kinematic variables, regardless of how constant the acceptance or A^0_{UU} are, then the solution is actually

$$p_{UU}(\phi) = \int d^D\boldsymbol{x}\; W_{UU}(\boldsymbol{x},\phi), \qquad p_{UT}(\phi,\phi_s) = \int d^D\boldsymbol{x}\; W_{UT}(\boldsymbol{x},\phi,\phi_s), \tag{33}$$

distinct from (at not equal to) the result for the other case (Equations 16 and 17).

Determining which interpretation is correct requires analysis of the flatness, with respect to all relevant variables, of W_{UU}, W_{UT}, and the acceptance. This is particularly challenging, since to interpret the estimate of W_{UU}, W_{UT} one must determine the flatness of W_{UU}, W_{UT}, and to determine said flatness, one must interpret an estimate of W_{UU}, W_{UT}. An iterative procedure may possibly be able to determine the flatness and correct interpretation, but such a method has yet to be determined.

Thus one can only use this correction method in a full multi-dimensional analysis with large data samples, and even then more work must be done to determine which (if any) of the above interpretations are valid.

2.2 Asymmetries

To determine the result analogous to that which extracts the asymmetries in the case of no acceptance, one uses

$$p_\pm = 1 \pm p_{UT}(\phi,\phi_s). \tag{34}$$

Setting the derivative equal to zero, analogous to Equation 29, results the expression

$$0 = \int d^D\boldsymbol{x} d\phi d\phi_s \left(\frac{dN_+}{p_+} - \frac{dN_-}{p_-}\right)\sin(\phi_s) \tag{35}$$

$$\propto \int d\phi d\phi_s \; \sin(\phi_s) \int d^D\boldsymbol{x}\; \epsilon(\boldsymbol{x},\phi,\phi_s) A^0_{UU}(\boldsymbol{x}) \frac{W_{UT}(\boldsymbol{x},\phi,\phi_s) - W_{UU}(\boldsymbol{x},\phi,\phi_s)p_{UT}(\phi,\phi_s)}{1 - p^2_{UT}(\phi,\phi_s)}. \tag{36}$$

The situation is equivalent to extracting the amplitudes. In the case that A^0_{UU}, W_{UU} and W_{UT} are not constant over the integration region, and yet the acceptance is constant, the solution is that of Equation 13. If instead W_{UU} and W_{UT} are constant, then the solution is

$$p_{UT} = \frac{\int d\boldsymbol{x}\; W_{UT}(\boldsymbol{x},\phi,\phi_s)}{\int d\boldsymbol{x}\; W_{UU}(\boldsymbol{x},\phi)}. \tag{37}$$

Note, when W_{UU} and W_{UT} are constant, the asymmetry equals

$$\begin{aligned}
\frac{\sigma_+ - \sigma_-}{\sigma_+ + \sigma_-} &= \frac{\int d\boldsymbol{x}\ A^0_{UU}(\boldsymbol{x}) W_{UT}(\boldsymbol{x},\phi,\phi_s)}{\int d\boldsymbol{x}\ A^0_{UU}(\boldsymbol{x}) W_{UU}(\boldsymbol{x},\phi)}, &(38)\\
&= \frac{\int d\boldsymbol{x}\ W_{UT}(\boldsymbol{x},\phi,\phi_s)}{\int d\boldsymbol{x}\ W_{UU}(\boldsymbol{x},\phi)} \frac{\int d\boldsymbol{x}\ A^0_{UU}(\boldsymbol{x})}{\int d\boldsymbol{x}\ A^0_{UU}(\boldsymbol{x})}, &(39)\\
&= \frac{\int d\boldsymbol{x}\ W_{UT}(\boldsymbol{x},\phi,\phi_s)}{\int d\boldsymbol{x}\ W_{UU}(\boldsymbol{x},\phi)}, &(40)
\end{aligned}$$

and thus the interpretation of both limits are the same.

Thus, the Normalization Monte Carlo method requires full multi-dimensional analysis with small bins in all variables for both extracting the asymmetry and amplitudes. However, the interpretation of the asymmetry moments is straight forward in both limits.

3 Acceptance Correction: Weight Method

One could also consider constructing an estimate of the acceptance function, denoted $\widehat{\epsilon}(\boldsymbol{x},\phi,\phi_s)$. This estimate would be purely from Monte Carlo data, and can be constructed as proportional to the ratio of the PDF of reconstructed (accepted) data over data in 4π. As this is Monte Carlo data, it should be possible to get enough data to produce a fine grained histogram or a KDE.

Let each event be weighted by a factor of $1/\widehat{\epsilon}(\boldsymbol{x},\phi,\phi_s)$, and let the PDF be $p_\pm$. The log-likelihood can then be written

$$L = \sum_{i=1}^{n_+} \frac{1}{\widehat{\epsilon}(\boldsymbol{x}^{(i)}_+, \phi^{(i)}_+, \phi^{(i)}_{s+})} \ln p_+(\phi^{(i)}_+, \phi^{(i)}_{s+}) + \sum_{j=1}^{n_-} \frac{1}{\widehat{\epsilon}(\boldsymbol{x}^{(j)}_-, \phi^{(j)}_-, \phi^{(j)}_{s-})} \ln p_-(\phi^{(j)}_-, \phi^{(j)}_{s-}) + \text{const}. \tag{41}$$

3.1 Amplitudes

Let $p_\pm$ be defined according to Equations 5, 14, 15. Taking the derivative with respect to the parameter b and proceeding as before yields

$$0 = \frac{\partial L}{\partial b} \propto \int d^D\boldsymbol{x} d\phi d\phi_s \ \left(\frac{dN_+}{\int dN_+} \frac{1}{\widehat{\epsilon} p_+} + \frac{dN_-}{\int dN_-} \frac{1}{\widehat{\epsilon}\ p_-} \right) \cos\phi. \tag{42}$$

Again assuming that the acceptance is top-bottom symmetric, the expression can be written

$$\begin{aligned}
0 &= \frac{1}{\int dN_\pm} \int d^D\boldsymbol{x} d\phi d\phi_s\ \cos(\phi)\ \frac{dN_\pm}{\widehat{\epsilon}\ p_\pm} &(43)\\
&\propto \frac{1}{\int dN_\pm} \int d\phi d\phi_s\ \cos(\phi)\ \int d^D\boldsymbol{x}\ \frac{\epsilon(\boldsymbol{x},\phi,\phi_s)}{\widehat{\epsilon}(\boldsymbol{x},\phi,\phi_s)} A^0_{UU}(\boldsymbol{x}) \frac{W_{UU}(\boldsymbol{x},\phi) \pm W_{UT}(\boldsymbol{x},\phi,\phi_s)}{p_{UU}(\phi) \pm p_{UT}(\phi,\phi_s)}. &(44)
\end{aligned}$$

Equivalently, taking the derivative with respect to the parameter a yields

$$\begin{aligned}
0 &= \frac{\partial L}{\partial a} &(45)\\
&\propto \int d^D\boldsymbol{x} d\phi d\phi_s\ \left(\frac{dN_+}{\int dN_+} \frac{1}{\widehat{\epsilon} p_+} - \frac{dN_-}{\int dN_-} \frac{1}{\widehat{\epsilon}\ p_-} \right) \sin(\phi_s) &(46)\\
&\propto \int d\phi d\phi_s\ \sin\phi_s \int d^D\boldsymbol{x}\ \frac{\epsilon(\boldsymbol{x},\phi,\phi_s)}{\widehat{\epsilon}(\boldsymbol{x},\phi,\phi_s)} A^0_{UU}(\boldsymbol{x}) \\
&\quad \times \left[\frac{W_{UU}(\boldsymbol{x},\phi) + W_{UT}(\boldsymbol{x},\phi,\phi_s)}{1 + p_{UT}(\phi,\phi_s)} - \frac{W_{UU}(\boldsymbol{x},\phi) - W_{UT}(\boldsymbol{x},\phi,\phi_s)}{1 - p_{UT}(\phi,\phi_s)} \right] &(47)\\
&\propto \int d\phi d\phi_s\ \sin\phi_s \int d^D\boldsymbol{x}\ \frac{\epsilon(\boldsymbol{x},\phi,\phi_s)}{\widehat{\epsilon}(\boldsymbol{x},\phi,\phi_s)} A^0_{UU}(\boldsymbol{x}) \frac{W_{UT}(\boldsymbol{x},\phi,\phi_s) p_{UU}(\phi) - W_{UU}(\boldsymbol{x},\phi) p_{UT}(\phi,\phi_s)}{p^2_{UU}(\phi,\phi_s) - p^2_{UT}(\phi,\phi_s)}. &(48)
\end{aligned}$$

Assuming that $\epsilon(\boldsymbol{x},\phi,\phi_s)/\widehat{\epsilon}(\boldsymbol{x},\phi,\phi_s) \approx 1$, the acceptance cancels and the solution is that of the desired interpretation, Equation 16, 17.

3.2 Amplitudes

Let $p_\pm$ be defined according to Equations 4, 5. By analogy to above, the derivative with respect to the parameter a yields

$$0 = \frac{\partial L}{\partial a} \propto \int d\phi d\phi_s \; \sin\phi_s \int d^D\boldsymbol{x} \; \frac{\epsilon(\boldsymbol{x},\phi,\phi_s)}{\widehat{\epsilon}(\boldsymbol{x},\phi,\phi_s)} A^0_{UU}(\boldsymbol{x}) \frac{W_{UT}(\boldsymbol{x},\phi,\phi_s) - W_{UU}(\boldsymbol{x},\phi) p_{UT}(\phi,\phi_s)}{1 - p^2_{UT}(\phi,\phi_s)}. \tag{49}$$

Again assuming $\epsilon(\boldsymbol{x},\phi,\phi_s)/\widehat{\epsilon}(\boldsymbol{x},\phi,\phi_s) \approx 1$, the acceptance likewise cancels and the solution is again that of the desired interpretation, Equation 13.

3.3 Conclusion

Asymmetry and amplitude moments can both be extracted using MLE, and depend on whether terms for the angular portion of the unpolarized cross section are included in the fit function. The Normalization Monte Carlo method of correcting for acceptance only works in specific limits. Each analysis should verify the applicability of the limits. In the case of extracting the asymmetry, the results can be directly interpreted as long as the limits are satisfied. For the amplitudes, however, the interpretation depends on exactly which limits are satisfied, something difficult to determine. Thus, it is likely that it never will be optimal to extracting amplitudes using the Normalization Monte Carlo method. A few specific, high data, multidimensional analyses may possibly find use to use this method.

However, the Weighting Method of correcting for acceptance works irregardless of whether and how the data is binned, and only depends on the accuracy of the estimate of the acceptance function. This second method is thus preferable, as it has a broad range of applicability, the limit is better satisfied (yielding more accurate interpretation of the results), and is easier to implement. The only drawback is that this method requires generating both the 4π and reconstructed Monte Carlo samples.

References

[1] `http://hermes.desy.de/cgi-bin/majord-show.cgi?dir=arch.closed/offline-list&msg=msg130408.0.txt`

[2] `http://hermes-wiki.desy.de/index.php/Fitting`

[3] An introduction to the Normalization Monte Carlo method is found in the note "Introduction to Maximum Likelihood Estimation," `http://www-hermes.desy.de/PLOTS/0908/sgliske/Gliske.Intro_to_MLE.pdf`